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Level sets estimation and Vorob'ev expectation of random compact sets

Philippe Heinrich and Radu Stefan Stoica and Viet Chi Tran*

June 27, 2011

Abstract

The issue of a “mean shape” of a random set X often arises, in particular in image analysis and pattern detection. There is no canonical definition but one possible approach is the so-called Vorob'ev expectation $\mathbb{E}_V(X)$, which is closely linked to quantile sets. In this paper, we propose a consistent and ready to use estimator of $\mathbb{E}_V(X)$ built from independent copies of X with spatial discretization. The control of discretization errors is handled with a mild regularity assumption on the boundary of X : a not too large ‘box counting’ dimension. Some examples are developed and an application to cosmological data is presented.

keywords: Stochastic geometry ; Random closed sets ; Level sets ; Vorob'ev expectation

AMS codes: Primary 60D05 ; Secondary 60F15 ; 28A80

1 Introduction and background

The present paper proposes a ready to use estimator based on level sets, and that allows to tackle the question of approximating the mean shape or expectation of a random set. The practical motivation of this work is given by pattern recognition applications coming from domains like astronomy, epidemiology and image processing [22, 23, 20, 19]. Several ways to define the expectation of a random set have been developed in the literature (see *e.g.* [14]). Our investigation leads us to the Vorob'ev expectation, closely related to quantiles and level-sets.

Let $(\Omega, \mathcal{A}, \mathbb{P})$ be a probability space. Consider a random compact set X in $[0, 1]^d$ as a map from Ω to the class \mathcal{C} of compact sets in $[0, 1]^d$ measurable in the following sense (see *e.g.* [14]):

$$\forall C \in \mathcal{C}, \quad \{\omega : X(\omega) \cap C \neq \emptyset\} \in \mathcal{A}.$$

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Robbins' formula, a straightforward consequence of Fubini's theorem, states that

$$\mathbb{E}\lambda(X) = \int_{[0,1]^d} \mathbb{P}(x \in X) \lambda(dx),$$

where λ is the Lebesgue measure. To define a “mean shape”, it is thus natural to consider the coverage function $p(x) = \mathbb{P}(x \in X)$. For $\alpha \in [0, 1]$, the (deterministic) α -level set of $p(x)$ is:

$$Q_\alpha = \{x \in [0, 1]^d : p(x) > \alpha\}$$

or $\{p > \alpha\}$ for short. Choosing α such that the volume of Q_α matches the mean volume of X provides the Vorob'ev expectation $\mathbb{E}_V(X)$ (see *e.g.* [5, 14, 15, 25]).

Definition 1.1. Set $F(\alpha) = \lambda(Q_\alpha) = \lambda\{p > \alpha\}$ and

$$\alpha^* = \inf\{\alpha \in [0, 1] : F(\alpha) \leq \mathbb{E}\lambda(X)\}.$$

The Vorob'ev expectation of X is a Borel set $\mathbb{E}_V(X)$ such that $\lambda(\mathbb{E}_V(X)) = \mathbb{E}\lambda(X)$ and

$$\{p > \alpha^*\} \subset \mathbb{E}_V(X) \subset \{p \geq \alpha^*\}. \quad (1)$$

Uniqueness of $\mathbb{E}_V(X)$ is ensured if F is continuous at α^* , and in this case one can choose $\mathbb{E}_V(X) = \{p \geq \alpha^*\}$ which is compact since $p(x)$ is upper semi-continuous. It can be shown ([15, Theorem 2.3. p.177]) that $\mathbb{E}_V(X)$ minimizes $B \mapsto \mathbb{E}\lambda(B \triangle X)$ under the constraint $\lambda(B) = \mathbb{E}\lambda(X)$, where $B \triangle X$ is the symmetric difference of B and X .

Despite their very natural definitions, neither the Q_α 's nor $\mathbb{E}_V(X)$ are tractable for applications. First, the coverage probability $p(x)$ is not always available in an analytical closed form. Second, level sets can not be computed for all the points $x \in [0, 1]^d$ and discretization should be considered.

The first point has been tackled by a large literature: plug-in estimators obtained by replacing $p(x)$ with

an empirical counterpart have been considered by Molchanov [10, 11, 13], Cuevas *et al.* [2, 3]. In particular, the latter establishes consistency of plug-in estimators for the L^1 -norm under weak assumptions. In particular, the function $p(x)$ needs not being continuous.

The aim of this paper is to derive a consistent and implementable estimator $K_{n,r}$, based on n i.i.d. copies X_1, \dots, X_n of X and spatial discretizations with a grid of mesh r . We extend proofs of consistency of plug-in estimators to estimators including a grid discretization, and generalize existing works on level-sets for the Vorob'ev expectation, when the level α is replaced by a level α^* that depends on X . We prove strong consistency for the symmetric difference and provide also convergence rates.

2 Estimation of level sets

2.1 Plug-in estimation of level sets

To define the plug-in estimators for sets Q_α , let us consider the empirical counterparts of $p(x)$:

$$p_n(x) = \frac{1}{n} \sum_{i=1}^n \mathbf{1}_{\{x \in X_i\}}.$$

Then, the plug-in estimator is

$$Q_{n,\alpha} = \{p_n > \alpha\}.$$

In the literature, several distances can be used for closed sets. Here, we are interested in the pseudo-distance defined for any $A, B \in \mathcal{B}([0, 1]^d)$ by $d(A, B) = \lambda(A \Delta B)$. Other possibilities are the Hausdorff distance, for which similar consistency results can be obtained, under additional assumptions on the regularity of $p(x)$ (see *e.g.* [11] and [3, Th. 1 and 2]). In [10, 11] for instance, $p(x)$ is assumed continuous. The case where $p(x)$ is a density function has also been much investigated. Kernel estimators may be used in the plug-in estimation. Rates of convergence [13, 16, 26] or asymptotic normality [9] are considered with regularity assumptions on $p(x)$. Adaptive estimation can also be performed [18].

L^1 -consistency is of practical interest and we follow the approach developed for instance in [3], and generalize their results with grid approximations in view of numerical implementation. For applications, we also aim at weak assumptions, in particular, the continuity of

the coverage function $p(x)$ should not be required. As a result, the function F is càdlàg with possible plateaus (constant regions). Note that F is the survival function of the random variable $p(U)$ with U uniformly distributed on $[0, 1]^d$.

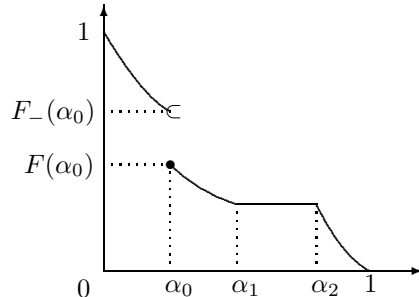


Figure 1: Behavior of function $F(\alpha) = \lambda(Q_\alpha)$

As an example, Figure 1 shows how the function F may look like. It can be observed that the plateaus of $p(x)$ make the discontinuities of F while the discontinuities of $p(x)$ provide the plateaus of F . The jump of F at α_0 corresponds to the Lebesgue measure of the points with coverage probability equal to α_0

$$F_-(\alpha_0) - F(\alpha_0) = \lambda\{p = \alpha_0\}.$$

The plateau $[\alpha_1, \alpha_2]$ of F means that the set of points with coverage probability between α_1 and α_2 is λ -negligible and $\lambda\{p > \alpha_1\} = \lambda\{p > \alpha\}$ for all $\alpha \in [\alpha_1, \alpha_2]$.

2.2 Grid approximation of a level set

The plug-in estimators $Q_{n,\alpha}$ are not satisfactory in view of applications, because they require computation of $p_n(x)$ for all x . In all what follows, r is a mesh introduced to work in $[0, 1]^d \cap r\mathbb{Z}^d$ rather than in $[0, 1]^d$. We seek for a candidate $Q_{n,\alpha}^r$ close to $Q_{n,\alpha}$ for small r , but less greedy in computations.

Definition 2.1. For any Borel set B in $[0, 1]^d$ and $r \in 2^{-\mathbb{N}}$, we call “grid approximation of B ” the set

$$B^r = \bigsqcup_{x \in B \cap r\mathbb{Z}^d} [x, x+r)^d.$$

As expected, some regularity of the border ∂B has to be introduced (see [4, p.38-39]):

Definition 2.2. Let

$$N_r(\partial B) = \text{Card}\{x \in r\mathbb{Z}^d : [x, x+r)^d \cap \partial B \neq \emptyset\}.$$

The “upper box counting dimension” of ∂B is

$$\overline{\dim_{\text{box}}}(\partial B) = \limsup_{r \rightarrow 0} \frac{\log N_r(\partial B)}{-\log r}.$$

A straightforward consequence of these definitions is:

Proposition 2.3. *Assume that $\overline{\dim_{\text{box}}}(\partial B) < d$. For all $\varepsilon > 0$, there exists r_ε such that*

$$0 < r < r_\varepsilon \implies d(B^r, B) \leq r^{d - \overline{\dim_{\text{box}}}(\partial B) - \varepsilon}.$$

The following result extends the result of Cuevas *et al.* [3, Th. 3] by adding a discretization scheme:

Proposition 2.4. *Assume that $\overline{\dim_{\text{box}}}(\partial X) \leq d - \kappa$ with probability one for some $\kappa > 0$. For all α such that $\lambda\{p = \alpha\} = 0$,*

(i) *with probability 1,*

$$\lim_{\substack{r \rightarrow 0 \\ n \rightarrow \infty}} d(Q_{n,\alpha}^r, Q_\alpha) = 0.$$

(ii) *for all $\varepsilon > 0$,*

$$\mathbb{E} d(Q_{n,\alpha}^r, Q_\alpha) \leq r^\kappa + 2e^{-2n\varepsilon^2} + F(\alpha - \varepsilon) - F(\alpha + \varepsilon).$$

3 Estimation of $\mathbb{E}_V(X)$: Kovyazin’s mean

Let us consider the volume $F_n(\alpha) = \lambda\{p_n > \alpha\}$. Following the approach of [5], we introduce first the empirical volume

$$\Lambda_n = \frac{1}{n} \sum_{i=1}^n \lambda(X_i),$$

and next

$$\alpha_n^* = \inf\{\alpha \in [0, 1] : F_n(\alpha) \leq \Lambda_n\}.$$

Definition 3.1. *The “Kovyazin’s mean” is a Borel set K_n defined by an empirical version of (1):*

$$\lambda(K_n) = \Lambda_n \quad \text{and} \quad \{p_n > \alpha_n^*\} \subset K_n \subset \{p_n \geq \alpha_n^*\}.$$

The following revisits the approach of Kovyazin [5]:

Theorem 3.2. *Assume that $\lambda\{p = \alpha^*\} = 0$. Then, with probability one,*

$$d(K_n, \mathbb{E}_v(X)) \xrightarrow{n \rightarrow \infty} 0.$$

3.1 A grid approximation of K_n

Let us consider the grid $[0, 1]^d \cap r\mathbb{Z}^d$. A first idea could be to take the grid approximation of $B = X$ or $B = K_n$, but this would provide a set B^r with mean volume not necessarily equal to Λ_n . Instead, we set

$$\alpha_{n,r}^* = \inf\{\alpha \in [0, 1] : \lambda(\{p_n > \alpha\}^r) \leq \Lambda_n\} \quad (2)$$

and consider a Borel set $K_{n,r}$ of volume Λ_n such that

$$\{p_n > \alpha_{n,r}^*\}^r \subset K_{n,r} \subset \{p_n \geq \alpha_{n,r}^*\}^r. \quad (3)$$

The set $K_{n,r}$ is the implementable estimator that we propose. Its definition amounts in the following procedure. First, we approximate the expected volume of the random set X by Λ_n , which gives the number of cells to select. The latter are chosen according to their estimated coverage, which is given by $p_n(x)$ for the cell $[x, x+r)^d$ with $x \in r\mathbb{Z} \cap [0, 1]^d$. The consistency and convergence rate are provided by the following results.

3.2 Consistency of $K_{n,r}$

Recall the definition of α^* in Definition 1.1 and set

$$\beta^* = \sup\{\alpha \in [0, 1] : F(\alpha) \geq \mathbb{E}\lambda(X)\}. \quad (4)$$

Our main theorem states that:

Theorem 3.3. *Assume that*

- (i) $\mathbb{P}(\overline{\dim_{\text{box}}}(\partial X) \leq d - \kappa) = 1$ for some $\kappa > 0$.
- (ii) *The Lebesgue measures of $\{p = \alpha^*\}$ and $\{p = \beta^*\}$ are zero.*

With probability one,

$$d(K_{n,r}, \mathbb{E}_V(X)) \xrightarrow[\substack{n \rightarrow \infty \\ r \rightarrow 0}]{} 0.$$

For the proof, we write that

$$d(K_{n,r}, \mathbb{E}_V(X)) \leq d(K_{n,r}, K_n) + d(K_n, \mathbb{E}_V(X))$$

and use Theorem 3.2 and the two following lemmas to conclude.

Lemma 3.4. *Assume that $\mathbb{P}(\overline{\dim_{\text{box}}}(\partial X) \leq d - \kappa) = 1$ for some $\kappa > 0$. Then, with probability one*

$$\alpha^* \leq \liminf_{\substack{n \rightarrow \infty \\ r \rightarrow 0}} \alpha_{n,r}^* \leq \limsup_{\substack{n \rightarrow \infty \\ r \rightarrow 0}} \alpha_{n,r}^* \leq \beta^*,$$

and as a sort of particular case, we also have

$$\alpha^* \leq \liminf_{n \rightarrow \infty} \alpha_n^* \leq \limsup_{n \rightarrow \infty} \alpha_n^* \leq \beta^*.$$

Lemma 3.5. *Assume $\mathbb{P}(\overline{\dim_{\text{box}}}(\partial X) \leq d - \kappa) = 1$ for some $\kappa > 0$. With probability one,*

$$\limsup_{\substack{n \rightarrow \infty \\ r \rightarrow 0}} d(K_{n,r}, K_n) \leq 2 \left[\lim_{\substack{\alpha \rightarrow \alpha^* \\ \alpha < \alpha^*}} F(\alpha) - F(\beta^*) \right].$$

4 Some examples

4.1 The region covered by a boolean model

As an example of multi-dimensional random set, let us consider the Boolean model [6, 12, 24], constructed as follows. First, take a Poisson point process Π_μ in \mathbb{R}^d ; the parameter μ is a locally finite measure on \mathbb{R}^d called intensity measure. Next consider a sequence of i.i.d compact sets $(\Xi_x)_{x \in \mathbb{R}^d}$, which is independent of Π_μ . Finally, replace each point x of Π_μ by the shifted corresponding set $x + \Xi_x$. The resulting union set

$$\Xi = \bigcup_{x \in \Pi_\mu} (x + \Xi_x)$$

is the Boolean model. The points x are called germs and the random set Ξ_0 is the ‘typical’ grain of the model. The Boolean model is also called the Poisson germ-grain model. To avoid trivial models where $\Xi = \mathbb{R}^d$ almost surely, the d -th moment of the radius of the circumscribed circle of Ξ_0 must be finite.

The distribution of the Boolean model is uniquely determined by its capacity functional (see [12, 24])

$$T_\Xi(C) = \mathbb{P}(\Xi \cap C \neq \emptyset) = 1 - \exp \left[-\mathbb{E}\mu(\check{\Xi}_0 \oplus C) \right], \quad (5)$$

where C ranges over compact sets in \mathbb{R}^d , $\check{\Xi}_0$ is the symmetric of typical grain with respect to the origin and \oplus the Minkowski addition.

Assume that the Boolean model is observed through the window $[0, 1]^d$ so that we focus on the random compact set

$$X = \Xi \cap [0, 1]^d,$$

that is the covered region in the cube by Ξ . That X is indeed compact requires some (known) work. Briefly, if Ξ is viewed as a random counting measure on the class \mathcal{C} of compact sets in \mathbb{R}^d , its intensity measure will be locally finite if and only if $\mathbb{E}\mu(\check{\Xi}_0 \oplus C) < \infty$ for every compact C . In these conditions, only finitely many sets $x + \Xi_x$ will hit the cube $[0, 1]^d$ almost surely (see [17, sections 3 and 4]).

4.1.1 Stationary case

This type of Boolean model refers to a translation-invariant intensity measure μ on \mathbb{R}^d so that $\mu(dx) = m\lambda(dx)$ for some $m > 0$. In the following, the considered grains Ξ_x are balls of random radius R such that $\mathbb{E}(R^d) < \infty$. The coverage probability $p(x)$ of X is obtained from (5) by taking $C = \{x\}$ with $x \in [0, 1]^d$:

$$p(x) = T_\Xi(\{x\}) = 1 - \exp \left[-m\lambda(B(0, 1))\mathbb{E}(R^d) \right].$$

Set for short $c_{m,d} = 1 - \exp \left[-m\lambda(B(0, 1))\mathbb{E}(R^d) \right]$. Since $p(x)$ is the constant $c_{m,d}$, it’s easy to conclude that

$$F(\alpha) = \mathbf{1}_{[0, c_{m,d})}(\alpha) \quad \text{and} \quad \alpha^* = c_{m,d}.$$

Thus, $Q_{\alpha^*} = \emptyset$ while $Q_{\alpha^* - \varepsilon} = [0, 1]^d$ for any $\varepsilon > 0$. In this case, $\mathbb{E}_v(X)$ is not unique and any measurable set with volume $\mathbb{E}\lambda(X)$ is a possible Vorob’ev expectation. Also, the assumption $\lambda\{p = \alpha^*\} = 0$ does not hold here and neither does Theorem 3.2.

4.1.2 Non-stationary case

This type of Boolean model may be obtained for locally finite intensity measures $\mu(dx) = m(x)\lambda(dx)$ with a non-constant positive function $m(x)$. We assume that the radius probability distribution $\mathbb{P} \circ R^{-1}$ admits a continuous density g with respect to the Lebesgue measure such that

$$\forall x \in [0, 1]^d, \quad \int_{[0, 1]^d} g(|x - y|) \frac{x - y}{|x - y|} \mu(dy) \neq 0. \quad (6)$$

The coverage probability of X requires the computation of the function

$$\begin{aligned} \phi(x) &= \mathbb{E}\mu \left(\check{\Xi}_0 \oplus \{x\} \right) \\ &= \mathbb{E}\mu \left(x + B(0, R) \right) \\ &= \int_{[0, 1]^d} \mathbb{P}(R > |x - y|) \mu(dy). \end{aligned}$$

For $\alpha \in (0, 1)$, the level set Q_α consists of points x satisfying:

$$\begin{aligned} p(x) > \alpha &\Leftrightarrow \exp(-\phi(x)) < 1 - \alpha \\ &\Leftrightarrow \phi(x) > \ln \left(\frac{1}{1 - \alpha} \right). \end{aligned}$$

Computing the gradient $\nabla_x \mathbb{P}(R > |x - y|)$ for $x \neq y$ gives the integrand of (6). Since g is continuous, ϕ is of class \mathcal{C}^1 with the non-vanishing derivative (6). Moreover, the boundary ∂Q_α coincide with the set $\{p = \alpha\}$ and is obtained as the solution of

$$\phi(x) = \ln \left(\frac{1}{1 - \alpha} \right).$$

Using the implicit function theorem, the boundary of Q_α is a \mathcal{C}^1 -manifold of dimension $d - 1$: it can be locally parameterized by \mathcal{C}^1 -functions of $d - 1$ variables. Assumption $\lambda\{p = \alpha\} = 0$ is satisfied. In this case, Proposition 2.4 holds for any $\alpha \in (0, 1)$ and Theorems 3.2 and 3.3 apply, which yields consistency and a rate of convergence for the estimator $K_{n,r}$.

4.1.3 Boolean model with atoms

In this section, we provide an example where the coverage function exhibits discontinuities. Consider the model Ξ of Section 4.1.2 with in addition an independent random vector (U_1, \dots, U_N) of independent Bernoulli random variables. Fix points y_1, \dots, y_N in $[0, 1]^d$ and $r_0 > 0$ and set

$$\Upsilon = \Xi \cup \bigcup_{i:U_i=1} B(y_i, r_0).$$

We have thus added a random union of deterministic balls to the model Ξ . In the case where some of the $\mathbb{P}(U_i = 1)$ are equal to 1, this model is reminiscent of the conditional Boolean model (see Lantuéjoul [6]). The coverage probability of $X = \Upsilon \cap [0, 1]^d$ is:

$$p(x) = 1 - e^{-\phi(x)} \prod_{i:B(y_i, r_0) \ni x} \mathbb{P}(U_i = 0).$$

and $p(x) > \alpha$ is equivalent to

$$\phi(x) - \sum_{i:B(y_i, r_0) \ni x} \ln \mathbb{P}(U_i = 0) > \ln \left(\frac{1}{1-\alpha} \right). \quad (7)$$

Set $\mathcal{D} = \cup_{i=1}^N \partial B(y_i, r_0)$. If we work on each connected component of $[0, 1]^d \setminus \mathcal{D}$, the sum in the l.h.s. of (7) is constant and we are reduced to the case considered in Section 4.1.2. Besides, $p(x)$ is discontinuous on the set \mathcal{D} . Thus $F(\alpha)$ exhibits plateaus. If $p(x)$ is continuous at α^* , then the Vorob'ev expectation is unique and consistency and rate of convergence can be obtained for $K_{n,r}$. Else $p(x)$ is discontinuous at α^* and there is no uniqueness of the Vorob'ev expectation.

4.2 Example on real data

The filamentary network is one of the most important features in studying galaxy distribution [8]. The point field in Figure 2 is given by the galaxy centers of the NGP150 sample obtained from the 2 degree Field Galaxy Redshift Survey (2dFGRS) [1]. It can be easily noticed that the galaxy positions are not spread uniformly in the observation window and the filamentary structure is observable simply by eye investigation.

The automatic delineation of these structure is an important challenge for the cosmological community. The authors in [22, 23] models these filamentary structures by a cloud X of interacting cylinders $C(x, \eta)$ which are encoded by their centers $x \in K$ compact subset of \mathbb{R}^3 and their directions $\eta \in \mathbb{S}_+^3$ the unit sphere with positive z -ordinate. To obtain such an object,

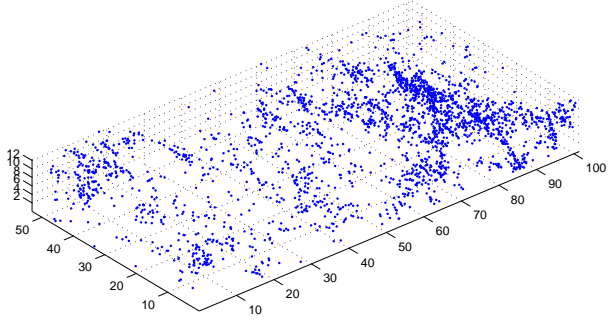


Figure 2: NGP150 sample from the 2dFGRS survey.

these authors use a point process Γ in $\mathbb{R}^3 \times \mathbb{S}_+^3$ which has density

$$h(\gamma|\theta) = \frac{\exp[-U_d(\gamma|\theta) - U_i(\gamma|\theta)]}{\alpha(\theta)}, \quad (8)$$

with respect to the Poisson point process Π_μ on $\mathbb{R}^3 \times \mathbb{S}_+^3$ with the Lebesgue measure as intensity μ . The energy function of the model is given by the sum of two terms that depend on parameters $\theta \in \Theta$ a compact subset of \mathbb{R}^m . The term $U_d(\gamma|\theta)$ depends on the observed galaxy fields and is called the data energy. It expresses that the point process giving the centers x is spatially inhomogeneous: more points will be drawn in region where observations are dense. The term $U_i(\gamma|\theta)$ is called the interaction energy and it is related to the connection and the alignment of the cylinders forming the pattern.

The random set that is considered is hence:

$$X = X(\Gamma) = \left(\bigcup_{(x,\eta) \in \Gamma} C(x, \eta) \right) \cap K.$$

For full complete details concerning the model and the simulation dynamics, the reader should refer to in [22, 23]. To fit our previous developed framework, the compact K should be chosen as (or imbedded in) $[0, 1]^d$ by using homothetical scaling of the data. But this is completely inessential.

The model (8) behaves as follows. If only the interaction energy is used, the model simulates a connected network which is independent of the data. If only the data term is used the model locates the filamentary regions but the cylinders are clustering in a disordered way and they neither connect nor form a network. The data energy acts as a non-stationary Poisson marked point process. The interaction energy acts as distance based pair-wise interaction

marked point process and it plays the role of a regularization term or a prior for the filamentary network.

Heuristically, the idea in [22, 23] is to estimate the parameter θ , which is unknown, and simulate realizations of X from which information on the distribution of X can be obtained. For instance, if X_1, \dots, X_n are realizations of X , their Vorob'ev mean can help us identify the patterns of the filamentary network by providing a mean shape appearing under the distribution of X . Tuning a model as (8) is not always a very simple task. Stoica et al. use a Bayesian frameworks and introduce a prior $\varrho(\theta)$ for the model parameters. Using a Metropolis-Hastings algorithm, throwing the burn-off period away and choosing simulations that are sufficiently distant, they generate a non-correlated sequence $(\theta_i, X_i)_{i \in \{1, \dots, n\}}$ that should be identically distributed if the algorithm converged correctly. The Metropolis-Hastings algorithm uses simulated annealing and depends on a temperature parameter T , and several strategies can be applied.

Once this is done, notice that the coverage function writes as:

$$p(x) = \mathbb{E} \left(\int_{\Theta} \mathbf{1}_{\{x \in X(\Pi_\mu)\}} h(\Pi_\mu | \theta) \varrho(\theta) d\theta \right). \quad (9)$$

The Lebesgue measure of the level sets induced by (9) is given by the function

$$F(\alpha) = \int_K \mathbf{1}_{\{p(x) > \alpha\}} \lambda(dx).$$

Since, $p(x)$ is not available in closed analytical form it is not a trivial task to check the continuity of $F(\alpha)$ to check if we are in the assumptions of Theorem 3.3.

4.2.1 Fixed temperature

If the temperature remains constant during the Metropolis-Hastings algorithm, then the algorithm is expected to produce a sequence of non-correlated random variables (θ_i, Γ_i) with density $h(\gamma | \theta) \varrho(\theta)$. The sequence $(X_i)_{i \in \{1, \dots, n\}}$ is then considered to be identically distributed.

The first empirical test consists in running the simulation dynamics at fixed temperature $T = 1$, and we simulate a sequence of $n = 1000$ realizations of X . The Monte Carlo counter-part of $F(\alpha)$ is shown in Figure 3. No observable discontinuity can be detected by simple visual inspection. Hence, using the same samples we obtain the empirical values $\Lambda_n = 1158$ and $\alpha_n^* = 0.36$.

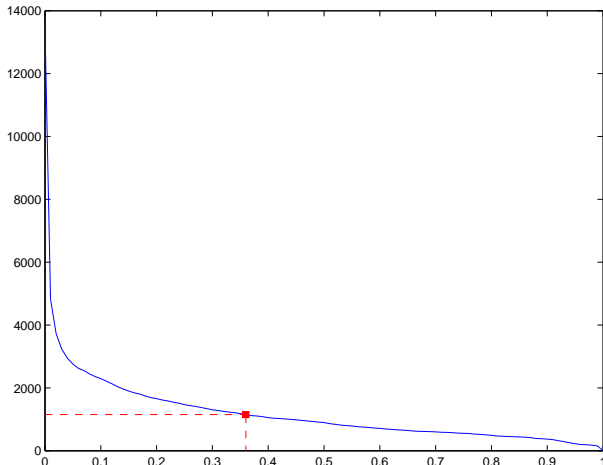


Figure 3: Monte-Carlo computation of the function $F(\alpha)$ for the galaxy catalogue NGP150 using a simulation dynamics at fixed temperature.

The estimator of the Vorob'ev expectation is shown in Figure 4. Even if running the simulation dynamics at fixed temperature does not provide an estimator of the filamentary pattern, the estimator of the Vorob'ev expectation can be used to assess the presence of a filamentary pattern in the data under the assumption that the model parameters are correct. The empirical computation of the sufficient statistics of the model can be also used in order to validate the presence of the filamentary pattern and also to give a more detailed morphological description [20, 22, 23].

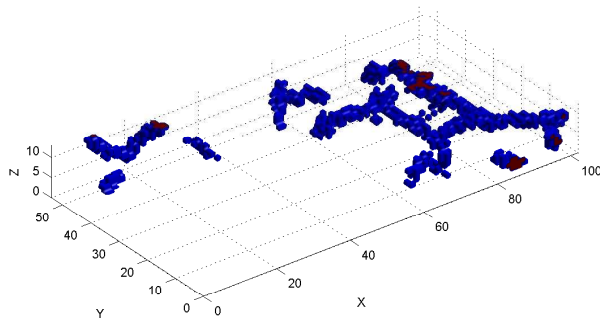


Figure 4: Estimator of the Vorob'ev expectation for the galaxy catalogue NGP150 using a simulation dynamics at fixed temperature.

4.2.2 Decreasing temperature

We now start with a low temperature T_0 and choose the cooling schedule along the Metropolis-Hastings algorithm as

$$T_n = \frac{T_0}{\log n + 1}. \quad (10)$$

Under these circumstances, the sequence $(\theta_i, \Gamma_i)_{i \in \{1, \dots, n\}}$ can be considered as non-correlated random variables that are uniformly distributed on the set maximizing the joint probability density or minimizing the total energy of the system (see [21])

$$\begin{aligned} (\hat{\theta}, \hat{\gamma}) &= \arg \max_{\Omega \times \Theta} h(\gamma|\theta) \varrho(\theta) \\ &= \arg \min_{\Omega \times \Theta} \left\{ \frac{U_{\mathbf{d}}(\gamma|\theta) + U_i(\gamma|\theta)}{\alpha(\theta)} - \log \varrho(\theta) \right\} 1, \end{aligned}$$

where Ω denotes the set of simple point measures on $\mathbb{R}^3 \times \mathbb{S}_+^3$. Clearly, the solution we obtain is not unique.

The second test was to obtain $n = 1000$ samples using the simulated annealing algorithm with $T_0 = 1$. The approximated $F(\alpha)$ function is shown in Figure 5. Comparing with the previous case, the function $F(\alpha)$ looks less smooth. Two other approximations are done. First, the simulated annealing simulates a non-homogeneous Markov chain. Second, the cooling schedule fixes the sequence of distributions converging towards the uniform distribution on the configuration sub-space maximizing $h(\gamma|\theta) \varrho(\theta)$. Again using the same samples we obtain the empirical values $\Lambda_n = 1730.6$ and $\alpha_n^* = 0.64$.

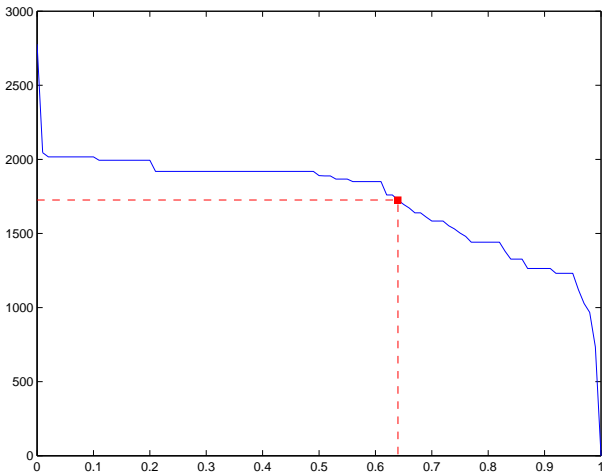


Figure 5: Computation of the function $F(\alpha)$ for the galaxy catalogue NGP150 using a simulated annealing algorithm.

The estimator of the Vorob'ev expectation computed using the simulated annealing algorithm is shown in Figure 6. Comparing with the first experience, the filamentary pattern has a bigger volume. As a consequence, this method is more useful for detecting average patterns of the filaments, while one would prefer the method with fixed temperature for estimation.

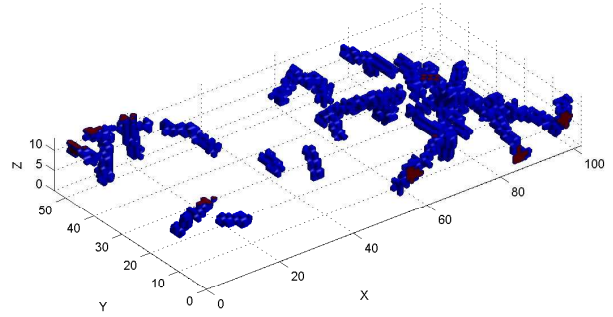


Figure 6: Estimator of the Vorob'ev expectation for the galaxy catalogue NGP150 using a simulated annealing algorithm.

The presented applications lead towards new questions concerning the level sets estimators. The first question consists in determining a class of models that allow computation of level sets and Vorob'ev expectation in the setting of this paper. A very intuitive answer leads to the following recommendations of using continuous intensity functions and interaction potentials. Clearly, this may be a quite restrictive condition. Hence, the second question would be whether continuous priors on the model parameter guarantee an appropriate behavior of the $F(\alpha)$ function. And finally a third question is whether there exists an optimal cooling schedule guaranteeing the working hypotheses for the construction of level sets based estimators. From our experiments, it seems for instance that constant temperature is good for estimating parameters while simulated annealing is better to detect patterns.

A Appendix: Proofs

Several times, the Strong Law of Large numbers in the separable Banach space $L^1([0, 1]^d)$ (L^1 SLLN) will be used (see *e.g.* [7, chap. 7]).

Proof of Proposition 2.3

It is not difficult to see that $B \triangle B^r$ is included in the union of cells $[x, x+r)^d$ ($x \in r\mathbb{Z}^d \cap [0, 1]^d$) that meet ∂B . As a result, we have

$$\lambda(B \triangle B^r) \leq N_r(\partial B)r^d.$$

Besides, given $\varepsilon > 0$, we get from definition (2.2) that for r small enough,

$$N_r(\partial B) \leq r^{-\overline{\dim_{\text{box}}}(\partial B) - \varepsilon}.$$

These two inequalities provide the result.

Proof of Lemma 3.4

Consider $\alpha < \alpha^*$ such that F is continuous at α . We show that

$$\mathbb{P}\left(\alpha \leq \liminf_{\substack{n \rightarrow \infty \\ r \rightarrow 0}} \alpha_{n,r}^*\right) = 1.$$

Otherwise, on a set of positive probability, we have $\alpha > \liminf_{\substack{n \rightarrow \infty \\ r \rightarrow 0}} \alpha_{n,r}^*$ and there exists a sequence $(n_k, r_k)_{k \geq 1}$ with $n_k \rightarrow \infty$ and $r_k \rightarrow 0$ such that $\alpha > \alpha_{n_k, r_k}^*$. Then, from the definition (3),

$$\begin{aligned} \Lambda_{n_k} &= \lambda(K_{n_k, r_k}) \\ &\geq \lambda(\{p_{n_k} > \alpha\}^{r_k}) \\ &\geq \lambda(\{p_{n_k} > \alpha\}) - d(\{p_{n_k} > \alpha\}^{r_k}, \{p_{n_k} > \alpha\}) \\ &\geq \lambda(\{p_{n_k} > \alpha\}) - \sup_n d(\{p_n > \alpha\}^{r_k}, \{p_n > \alpha\}). \end{aligned}$$

Note that $\partial\{p_n > \alpha\} \subset \bigcup_{i=1}^n \partial X_i$ since p_n is locally constant on the complementary of $\bigcup_{i=1}^n \partial X_i$. Moreover, since the ‘‘upper box-counting dimension’’ $\overline{\dim_{\text{box}}}(\cdot)$ has monotonic and stability properties (see [4]), we get whatever α , for the constant κ introduced in the assumptions,

$$\begin{aligned} \overline{\dim_{\text{box}}}(\partial\{p_n > \alpha\}) &\leq \overline{\dim_{\text{box}}}\left(\bigcup_{i=1}^n \partial X_i\right) \\ &= \max_{1 \leq i \leq n} \overline{\dim_{\text{box}}}(\partial X_i) \leq d - \kappa. \end{aligned}$$

It follows then from Proposition 2.3 that for k large enough,

$$\sup_n d(\{p_n > \alpha\}^{r_k}, \{p_n > \alpha\}) \leq r_k^{\kappa/2}, \quad (12)$$

and thus

$$\Lambda_{n_k} \geq \lambda\{p_{n_k} > \alpha\} - r_k^{\kappa/2}.$$

Taking the limit as $k \rightarrow \infty$ and invoking the L^1 -SLLN for $(p_n)_{n \geq 1}$, we obtain

$$\mathbb{E}\lambda(X) \geq \lambda\{p > \alpha\} = F(\alpha). \quad (13)$$

This contradicts the definition of α^* . As a consequence, we have

$$\mathbb{P}\left(\alpha^* \leq \liminf_{\substack{n \rightarrow \infty \\ r \rightarrow 0}} \alpha_{n,r}^*\right) = 1.$$

Very similarly, we can prove that

$$\mathbb{P}\left(\limsup_{\substack{n \rightarrow \infty \\ r \rightarrow 0}} \alpha_{n,r}^* \leq \beta^*\right) = 1.$$

The particular case without the mesh r is in the same spirit: we can show that there exists a sequence $n_k \rightarrow \infty$ such that $\Lambda_{n_k} \geq \lambda(\{p_{n_k} > \alpha\})$ which leads to (13).

Proof of Lemma 3.5

From $d(A, B) = \lambda(A) - \lambda(B) + 2\lambda(B \setminus A)$, and since $K_{n,r}$ and K_n have the same volume, we deduce

$$\begin{aligned} \frac{1}{2}d(K_{n,r}, K_n) &\leq \lambda(\{p_n \geq \alpha_{n,r}^*\}^r \setminus \{p_n > \alpha_n^*\}) \\ &\leq \lambda(\{p_n \geq \alpha_{n,r}^*\}^r \setminus \{p_n \geq \alpha_{n,r}^*\}) \\ &\quad + \lambda(\{p_n \geq \alpha_{n,r}^*\} \setminus \{p_n > \alpha_n^*\}) \\ &\leq d(\{p_n \geq \alpha_{n,r}^*\}^r, \{p_n \geq \alpha_{n,r}^*\}) \\ &\quad + \lambda\{\alpha_{n,r}^* \leq p_n \leq \alpha_n^*\}. \end{aligned}$$

The first term in the majoration is with probability one less than $r^{\kappa/2}$ for r small enough, as in (12). For the second one, let $\alpha < \alpha^*$ and $\beta > \beta^*$; by Lemma 3.4, there exists $n_{\alpha, \beta} \geq 1$ and $r_{\alpha, \beta} > 0$ such that for all $n \geq n_{\alpha, \beta}$ and $r \in (0, r_{\alpha, \beta})$,

$$\lambda\{\alpha_{n,r}^* \leq p_n \leq \alpha_n^*\} \leq \lambda\{\alpha < p_n \leq \beta\},$$

and again by the L^1 -SLLN for $(p_n)_{n \geq 1}$,

$$\lambda\{\alpha < p_n \leq \beta\} \xrightarrow[n \rightarrow \infty]{} \lambda\{\alpha < p \leq \beta\} = F(\alpha) - F(\beta),$$

provided F is continuous at α and β . We deduce that with probability one

$$\limsup_{\substack{n \rightarrow \infty \\ r \rightarrow 0}} d(K_{n,r}, K_n) \leq 2[F(\alpha) - F(\beta)],$$

and the proof is easily completed.

Proof of Theorem 3.2

Consider Borel sets A, B , $\alpha, \beta \in [0, 1]$ and coverage functions p, q such that

$$\{p > \alpha\} \subset A \subset \{p \geq \alpha\} \quad \text{and} \quad \{q > \beta\} \subset B \subset \{q \geq \beta\}.$$

From $d(A, B) = \lambda(A) - \lambda(B) + 2\lambda(B \setminus A)$, we deduce

$$\begin{aligned} d(A, B) &\leq |\lambda(A) - \lambda(B)| \\ &\quad + 2[\lambda\{p \geq \alpha, q \leq \beta\} \wedge \lambda\{p \leq \alpha, q \geq \beta\}], \end{aligned}$$

and for $A = K_n$ and $B = \mathbb{E}_V(X)$, we get

$$d(K_n, \mathbb{E}_V(X)) \leq |\Lambda_n - \lambda(\mathbb{E}_V(X))| + 2m_n \quad (14)$$

with

$$m_n = \lambda\{p_n \geq \alpha_n^*, p \leq \alpha^*\} \wedge \lambda\{p_n \leq \alpha_n^*, p \geq \alpha^*\}.$$

The first term in (14) converges a.s. towards 0 by the SLLN. The second one requires to distinguish two cases:

$\alpha^* = \beta^*$: It's enough to prove that, with probability one,

$$p_n - \alpha_n^* \xrightarrow[n \rightarrow \infty]{L^1([0,1]^d)} p - \alpha^*. \quad (15)$$

Indeed together with the assumption $\lambda\{p = \alpha^*\} = 0$ this yields

$$\lambda\{p_n - \alpha_n^* \leq 0, p \geq \alpha^*\} \rightarrow \lambda\{p - \alpha^* \leq 0, p \geq \alpha^*\} = 0,$$

and thus m_n tends to 0 as $n \rightarrow \infty$. But (15) stems from Lemma 3.4 that gives $\alpha_n^* \rightarrow \alpha^*$ with probability one and $p_n \xrightarrow[n \rightarrow \infty]{L^1([0,1]^d)} p$ also with probability one.

$\alpha^* < \beta^*$: We distinguish three subcases. If $\alpha_n^* < \alpha^*$, then

$$\begin{aligned} m_n &\leq \lambda\{p_n \leq \alpha_n^*, p \geq \alpha^*\} \\ &\leq \lambda\{p_n \leq \alpha_n^*, p \geq \beta^*\} + \lambda\{\alpha^* \leq p < \beta^*\} \\ &= \lambda\{p_n \leq \alpha_n^*, p \geq \beta^*\} \\ &\quad + \lambda\{p = \alpha^*\} + (F(\alpha^*) - F(\beta^* -)) \end{aligned}$$

The two last terms are zero, thus:

$$m_n \leq \lambda\{|p_n - p| \geq \beta^* - \alpha^*\} \leq \frac{\|p_n - p\|_{L^1}}{\beta^* - \alpha^*},$$

by using the Markov inequality. If $\alpha_n^* > \beta^*$, then starting from $m_n \leq \lambda\{p_n \geq \alpha_n^*, p \leq \alpha^*\}$ we obtain the same upper-bound. Finally, when $\alpha^* \leq \alpha_n^* \leq \beta^*$,

$$\begin{aligned} (\beta^* - \alpha^*)m_n &\leq (\beta^* - \alpha_n^*)\lambda\{p_n \leq \alpha_n^*, p \geq \beta^*\} \\ &\quad + (\alpha_n^* - \alpha^*)\lambda\{p_n \geq \alpha_n^*, p \leq \alpha^*\} \\ &\leq \|p_n - p\|_{L^1}. \end{aligned}$$

In the three cases, m_n is bounded by $\|p_n - p\|_{L^1}/(\beta^* - \alpha^*)$ which converges to zero a.s.

Proof of Proposition 2.4

By triangular inequality and Proposition 2.3,

$$\mathbb{E}d(Q_{n,\alpha}^r, Q_\alpha) \leq r^\kappa + \mathbb{E}d(Q_{n,\alpha}, Q_\alpha).$$

It remains to control the last term $\mathbb{E}d(Q_{n,\alpha}, Q_\alpha)$. We have

$$\begin{aligned} d(Q_{n,\alpha}, Q_\alpha) &= \lambda\{p_n > \alpha, p \leq \alpha\} + \lambda\{p_n \leq \alpha, p > \alpha\} \\ &\leq \lambda\{x \in [0, 1]^d : |p_n(x) - p(x)| \geq |p(x) - \alpha|\}. \end{aligned}$$

Taking expectation and using Fubini's theorem and Bernstein's inequality, one gets for all $\varepsilon > 0$

$$\begin{aligned} \mathbb{E}d(Q_{n,\alpha}, Q_\alpha) &\leq \int_{[0,1]^d} \mathbb{P}\{|p_n(x) - p(x)| \geq |p(x) - \alpha|\} \lambda(dx) \\ &\leq \int_{\{|\alpha - p| \geq \varepsilon\}} 2e^{-2n|\alpha - p(x)|^2} \lambda(dx) \\ &\quad + \int_{\{|\alpha - p| < \varepsilon\}} \lambda(dx) \\ &\leq 2e^{-2n\varepsilon^2} + F(\alpha - \varepsilon) - F(\alpha + \varepsilon). \end{aligned}$$

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